Superconductivity of the One-Dimensional d-p Model with p-p transfer

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Using the numerical diagonalization method, we investigate the one-dimensional d-p model, simulating a Cu-O linear chain with strong Coulomb repulsions. Paying attention to the effect of the transfer energy t_{pp} between the nearest neighbor oxygen-sites, we calculate the critical exponent of correlation functions K_ρ based on the Luttinger liquid relations and the ground state energy $E_0(\phi)$ as a function of an external flux ϕ. We find that the transfer t_{pp} increases the charge susceptibility and the exponent K_ρ in cooperation with the repulsion U_d at Cu-site. We also show that anomalous flux quantization occurs for $K_\rho > 1$. The superconducting region is presented on a phase diagram of U_d vs. t_{pp} plane.

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Low-dimensional strongly correlated electron systems attract much interest due to the possible relevance to high-T_c superconductivity. A considerable number of theoretical studies have been performed on the strongly correlated fermion models either in one-band or multi-band version to understand the mechanism of the high temperature superconductivity. However, there is no consensus on what the actual mechanism of the superconductivity is, except for the fact that the strong repulsive interaction on Cu-site plays an important role in the mechanism. [1,2] To achieve a solid understanding of this problem, some rigorous studies, even of the simplest models, are highly desirable at this stage. For such purpose, numerical diagonalization studies of finite size systems may be successful. [3–6] In particular, one-dimensional d-p model, simulating a Cu-O linear chain with strong Coulomb repulsions, provides a good target to investigate the mechanism of the high-T_c superconductivity. [7–14] The model contains hopping t_{pd} between Cu(d)-site and oxygen(p)-site and repulsive interaction at the d- and p-site (U_d and U_p, respectively). In addition, it can contain the nearest-neighbor d-p interaction U_{pd} and/or hopping t_{pp} between the nearest-neighbor p-sites.

In the previous work, [7–9] the present authors have studied the one-dimensional d-p model with large on-site Coulomb repulsion U_d at Cu-sites and inter-site repulsion U_{pd}, by using the numerical diagonalization method. With the help of the Luttinger liquid relations, the superconducting(SC) correlation is found to be dominant compared with the CDW and SDW correlations in the proximity of the phase separation. The SC phase appears for $1.0 \lesssim U_{pd} \lesssim 1.6$ almost independent of the filling with $1.3 \lesssim n \lesssim 1.7$. Near the half-filling $n = 1$ and the full-filling $n = 2$, however, the SC correlation is suppressed. [10] Recently, Sudbø et al. showed that the d-p chain with large U_{pd} exhibits flux quantization with charge $2e$ and slow algebraic decay of the singlet SC correlation function on oxygen sites. [11] Other studies of the d-p chain also showed that U_{pd} enhances the charge fluctuation as well as the SC fluctuations and when it exceeds a certain critical value the system becomes unstable towards phase separation. [12,13] All of these studies claimed that the parameter U_{pd} is central in inducing a SC state at $T = 0$.

However, if one adds the hopping term t_{pp} to the model, the situation will be changed completely. It enhances the charge fluctuation and increases the exponent K_ρ as the parameter U_{pd} does. Therefor, the repulsive interaction U_{pd} is not always necessary for the SC state. In the present paper, to clarify the effect of t_{pp}, we study the one-dimensional d-p model with the hopping t_{pp} by the numerical diagonalization. We calculate the critical exponent of correlation functions K_ρ and the ground state energy $E_0(\phi)$ as a function of an external flux ϕ. Using the results for the critical exponent, we show a SC region on the $U_d - t_{pp}$ plane.

We consider the following model Hamiltonian for the Cu-O chain:

$$H = t_{pd} \sum_{<ij>,\sigma} (p^\dagger_{i\sigma} d_{j\sigma} + h.c.) + t_{pp} \sum_{<ij>,\sigma} (p^\dagger_{i\sigma} p_{j\sigma} + h.c.) + \epsilon_d \sum_{j,\sigma} d^\dagger_{j\sigma} d_{j\sigma} + \epsilon_p \sum_{i,\sigma} p^\dagger_{i\sigma} p_{i\sigma} + U_d \sum_j n_{dj\uparrow} n_{dj\downarrow} \quad (1)$$

where $d^\dagger_{j\sigma}$ and $p^\dagger_{i\sigma}$ stand for creation operators of a hole with spin σ in the Cu(d)-orbital at site j and of a hole with spin σ in the O(p)-orbital at site i respectively, and $n_{dj\sigma} = d^\dagger_{j\sigma} d_{j\sigma}$. Here, t_{pd} stands for the transfer energy between the nearest neighbor d- and p-sites, which will be set to be unity (t_{pd}=1) hereafter in the present study. The atomic energy levels of d- and p-orbitals are given by ϵ_d and ϵ_p, respectively. The charge-transfer energy Δ is defined as $\Delta = \epsilon_p - \epsilon_d$.

To achieve systematic calculation, we use the periodic boundary condition for $N_h = 4m + 2$ and antiperiodic boundary condition for $N_h = 4m$, where N_h is the total hole number and m is an integer. This choice of the boundary condition removes accidental degeneracy so that the ground state might always be a singlet with zero momentum. The filling n is defined by $n = N_h/N_u$, where N_u is the total number of unit cells (each unit cell contains a d- and a p-orbitals) and the Fermi wave number k_F is given as $k_F = \frac{\pi}{2} n$.

We numerically diagonalize the Hamiltonian up to 12 sites (6unit cells) using the standard Lanczos algorithm.

The chemical potential $\mu(N_h, N_u)$ is defined by

$$\mu(N_h, N_u) = \frac{E_0(N_h+1, N_u) - E_0(N_h-1, N_u)}{2} \quad , \quad (2)$$

where $E_0(N_h, N_u)$ is the total ground state energy of a system with N_u unit cells and N_h holes. When the charge gap vanishes in the thermodynamic limit, the uniform charge susceptibility χ_c is obtained from

$$\chi_c(N_h, N_u) = \frac{2/N_u}{\mu(N_h+1, N_u) - \mu(N_h-1, N_u)} \quad (3)$$

In the Luttinger liquid theory, some relations have been established as universal relations in the one-dimensional models. [15–17] In the model which is isotropic in spin space, the critical exponents of various types of correlation functions are determined by a single parameter K_ρ, which is the exponent of the power-law decay of correlation functions. For the one-dimensional d-p model in the weak coupling regime, Matsunami and Kimura [20] calculated the critical exponents of some correlation functions by using the renormalization group analysis (g-ology), and shown that the system belongs to the Tomonaga-Luttinger (TL) liquid. In the present authors' recent work, [8] we have shown the numerical results of the critical exponent K_ρ and the phase diagram on the U_d-U_{pd} plane including the weak coupling region and the strong coupling region. In the weak coupling region, it agrees with the results of the g-ology. An analysis of spin-gap indicates that the strong coupling region also belongs to the TL regime and not to the Luther-Emery (LE) regime. Here, the LE regime is characterized by a gap of the spin excitation spectrum, while in the TL regime, the excitation is gapless. [17,18]

It is predicted that SC correlation is dominant for $K_\rho > 1$ (the correlation function decays as $\sim r^{-(1+\frac{1}{K_\rho})}$ in the TL regime and as $\sim r^{-\frac{1}{K_\rho}}$ in the LE regime), whereas Charge Density Wave (CDW) or Spin Density Wave (SDW) correlations is dominant for $K_\rho < 1$ (correlation functions decay as $\sim r^{-(1+K_\rho)}$ in the TL regime and as $\sim r^{-K_\rho}$ in the LE regime). In the TL regime, the singlet SC and triplet SC correlation functions have the same critical exponent apart from a logarithmic correction. On the other hand, in the LE regime, the correlation functions of SDW and triplet SC decrease exponentially. The parameter K_ρ is related to the charge susceptibility χ_c and the charge velocity v_c by the relations, [4,15,17,19]

$$K_\rho = \frac{\pi}{2} v_c \chi_c \quad (4)$$

with $v_c = \frac{N_u}{2\pi}(E_1 - E_0)$,where $E_1 - E_0$ is the lowest charge excitation energy. We can also determine the K_ρ by the Drude weight D

$$K_\rho = \frac{1}{2}(\pi \chi_c D)^{1/2} \quad (5)$$

with $D = \frac{\pi}{N_u}\frac{\partial^2 E(\phi)}{\partial \phi^2}$, where $E(\phi)$ is the total energy of the ground state as a function of flux ϕ. [17] Using these two independent equations of the K_ρ, we will check the consistency of the Luttinger liquid relations.

For a non-interacting system ($U_d = 0$), the Hamiltonian (1) is easily diagonalized and a dispersion relation is given as

$$E^{\pm}(k) = \frac{1}{2}\Big\{\epsilon_d + \epsilon_p + 2t_{pp}\cos k \pm \sqrt{(\Delta + 2t_{pp}\cos k)^2 + 16(t_{pd}\cos(k/2))^2}\Big\} \quad (6)$$

where k is a wave vector and $E^+(k)(E^-(k))$ represents a upper (lower) band energy. Compared with the case with $t_{pp} = 0$, the width of the lower band $E^-(k)$ becomes narrower for $t_{pp} > 0$. Note that it decreases with Δ and becomes perfectly flat at $\Delta = 2t_{pp} - t_{pd}^2/t_{pp}$. When one decreases Δ further, the band bends with a peak at $k = 0$. To investigate the band structure of interacting systems, we consider the chemical potential μ, which is corresponding to Fermi energy E_F at $T = 0$. Figure 1(a) shows μ as a function of the filling n for several values of U_d with $\Delta = 2$ and $t_{pp} = 0.5$. We calculate the value of μ by using eq.(2) at the hole densities $n = 5/4, 7/4, 7/5, 9/5, , 7/6, 9/6$ and $11/6$. Data points with $U_d = 0$ seem to sit closely along on the dispersion curve of $E^-(k_F)$. It suggests that the finite-size effect is sufficiently small.

When U_d is large, μ is large and weekly depends on n. Especially, the slope of μ becomes almost flat at $U_d = 6.5$. In this case, the charge susceptibility χ_c almost diverges, because of the relation, $\chi_c^{-1} = \frac{d\mu}{dn}$. The result suggests that the width of effective hole band becomes very narrow due to a strong correlation effect of large repulsion U_d. In order to see the behavior of the charge susceptibility more qualitatively, in Fig. 1(b), we show the inverse of the charge susceptibility χ^{-1} as a function of U_d in a system with 6 unit cells for $\Delta = 2$. In the case of $t_{pp} = 0$, the U_d-dependence of χ^{-1} is week and χ^{-1} remains as a finite value. On the other hand, it is close to zero at $U_d \simeq 6.75$ for $t_{pp} = 0.5$. It shows that the transfer t_{pp} increases the charge susceptibility in cooperation with the repulsion U_d. If we use the Hartree-Fock(H.F.) approximation, the atomic levels of d-orbitals ϵ_d are pushed up as $\tilde{\epsilon_d} = \epsilon_d + \frac{1}{2}U_d < n_d >$, where $< n_d >$ is the mean value of hole density n_d at a d-site and determined by solving the self-consistent equation of $< n_d >$. Then, the band structure is approximately described as a renormalized band $\tilde{E}(k)$ whose Δ is replaced by $\tilde{\Delta} = \Delta - \frac{1}{2}U_d < n_d >$. The band width of $\tilde{E}^-(k)$ decreases as $\tilde{\Delta}$ decreases and becomes zero at sufficiently large U_d. The decreases of the band width leads to the enhancement of χ_c as shown in Fig.1(b).

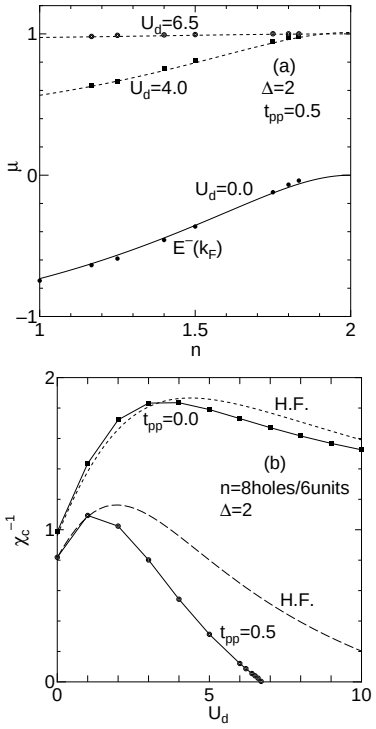

FIG. 1. (a) The chemical potential μ as a function of the filling n for various values of U_d. μ is calculated for N_u= 8, 10 and 12. The solid line represents $E^-(k_F)$. The broken lines are guide for eye. (b) The inverse charge susceptibility χ^{-1} as a function of U_d for $t_{pp} = 0.0$ and 0.5 with the results in the H.F. approximation.

Next, we show the critical exponent of correlation functions K_ρ as a function of U_d in Fig.2(a). We calculate K_ρ in two ways by using eq.(4) and eq.(5) independently, one is obtained by combining the charge velocity v_c and the charge susceptibility χ_c and the other is expressed by the Drude weight. The result shows that the values of K_ρ obtained by in the two different ways are well consistent with each other except for $U_d \lesssim -1$. We also show K_ρ obtained by the g-ology together in Fig.2(a). In the weak coupling regime, the results of numerical diagonalization are in good agreement with those of the g-ology. These results indicate that the Luttinger liquid theory can be applied to the one-dimensional d-p model successfully and finite-size effect of K_ρ is not so large.

To judge which of the two estimations of K_ρ is better from a point of view of finite-size effect, we watch the values of K_ρ at $U_d = 0$. The one from eq.(4) is equal to 0.972 and the other from eq.(5) is 1.002. Taking account of K_ρ being always equal to unity in noninteracting case, we infer that the estimation from eq.(5) is better than the other. Furthermore, the comparison of those values of K_ρ with the values obtained in the g-ology in the weak coupling regime also indicates that the estimation of K_ρ from eq.(5) gives a better result. Therefore, we will use the value of K_ρ expressed by eq.(5) in the following.

Fig.2(a) shows that K_ρ decreases as U_d increases when $U_d \lesssim 3$. However, K_ρ increases with U_d for $U_d \gtrsim 3$ and diverges at $U_d \sim 6.8$ where the charge susceptibility diverges. The divergence indicates that the width of the effective band $\tilde{E}^-(k)$ is close to zero. When K_ρ is larger than unity, the SC correlation is expected to be most dominant compared with CDW and SDW correlations. The region where $K_\rho > 1$ appears at $6.5 \lesssim U_d \lesssim 6.8$. It seems to be fairly small, but surely exists. To confirm the ground state to be in the SC state, we show the ground state energy $E_0(\phi)$ as a function of an external flux ϕ in Fig.2(b). The anomalous flux quantization occurs at $U_d = 6.7$, where K_ρ is about 2.0. When $U_d = 6.0$, K_ρ is less than unity and the anomalous flux quantization is not found. These results support that the SC phase really appears at $K_\rho > 1$.

Generally speaking, the SC phase is induced by an attractive interaction between quasi-particles. To examine the effective attraction, we introduce the repulsive interactions U_{dd} (U_{pp}) between the nearest-neighbor d-d (p-p) sites and the repulsion U_p. If those repulsions act between a relevant pair of holes or cancel the effective attraction, the SC state is expected to be suppressed and K_ρ is reduced. We find that U_{dd} does not affect K_ρ, but U_p ($\gtrsim 0.2$), as well as U_{pp}, decreases it. It suggests that the relevant pair of holes sit not on the d-sites but on the p-sites and the strength of the attraction is of order of 0.2. [21]

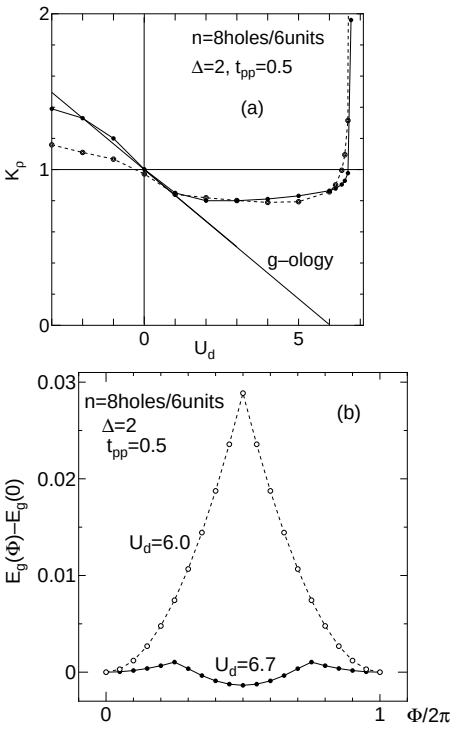

FIG. 2. (a) K_ρ as a function of U_d. The solid circles with the solid line represent the estimation from eq.(5) and the open circles with the broken line represent the estimation from eq.(4). (b) The energy difference $E_0(\phi) - E_0(0)$ as a function of an external fluxϕ.

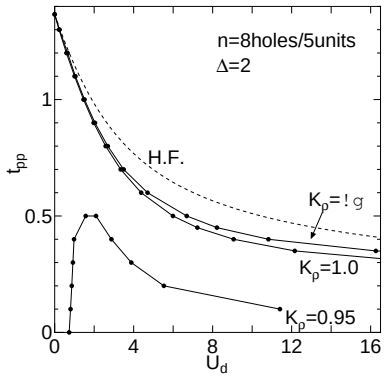

FIG. 3. Contour map for the K_ρ on the U_d-t_{pp} plane at $\Delta = 2$ for the 5-unit 8-hole system (n=8/5). The broken line represents t^c_{pp} obtained in the H.F. approximation.

Finally, we investigate the critical exponent K_ρ in detail and obtain the phase diagram in the $U_d - t_{pp}$ parameter plane. Figure 3 shows a contour map of K_ρ for $n = 8/5$ system. The region sandwiched between two lines with $K_\rho = 1$ and $K_\rho = \infty$ is corresponding to the SC region. The region is very small for small U_d, however, it increases with U_d.

In the H.F. approximation, the renormalized band $\tilde{E}^-(k)$ becomes flat at a critical value t^c_{pp} which is given as

$$t^c_{pp} = \frac{1}{4}\Big\{\Delta - \frac{1}{2}U_d < n_d > + \sqrt{(\Delta - \frac{1}{2}U_d < n_d >)^2 + 8t^2_{pd}}\Big\}.$$

Here, the approximation breaks down for $t_{pp} \geq t^c_{pp}$. We expect that the point of $t_{pp} = t^c_{pp}$ corresponds to that of $K_\rho = \infty$. In the noninteracting system ($U_d = 0$), $t^c_{pp} = \frac{1+\sqrt{3}}{2}$ for $\Delta = 2$. As U_d increases, t^c_{pp} decreases as shown in Fig.3. It seems that the line of t^c_{pp} is near that of $K_\rho = \infty$.

In summary, we have numerically diagonalized the one-dimensional d-p model with finite sizes. Paying special attention to the role of t_{pp}, we have calculated chemical potential and critical exponent K_ρ. We have also showed the anomalous flux quantization observed in the SC state. Using the Luttinger liquid relations, we have found that the SC correlation is dominant compared with the CDW and SDW correlations in the proximity of the parameter region where the renormalized band becomes flat. We have confirmed that t_{pp} enhances the charge fluctuation and promotes the SC correlation as U_{pd} does.

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